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Poly[μ_5-(4-methoxybenzenesulfonato)-sodium]

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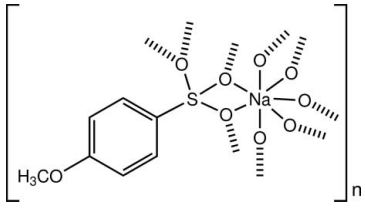
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.037; wR factor = 0.101; data-to-parameter ratio = 14.9.

In the title complex, $[Na(C_7H_7O_4S)]_n$, the Na^I ion is coordinated in a slightly distorted pentagonal-bipyramidal environment by seven O atoms [Na—O = 2.3198 (16)–2.5585 (17) Å]. The 4-methoxybenzenesulfonate anions act as bis-chelating and bridging ligands, forming a two-dimensional polymer parallel to (001), which is further linked into a three-dimensional network by weak C—H···O hydrogen bonds.

Related literature

For the appplications of aromatic sulfonic acids, see: Babu *et al.* (2003); Chanawanno *et al.* (2010); King (1991); Ruanwas *et al.* (2010); Schöngut *et al.* (2011); Siril *et al.* (2007); Taylor *et al.* (2006). For a related structure, see: Smith *et al.* (2004). For standard bond-lengths, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Na(C_7H_7O_4S)]$
M_r = 210.19
Orthorhombic, *Pbca*
a = 8.3121 (8) Å
b = 6.0287 (6) Å
c = 35.930 (3) Å
V = 1800.5 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.38 mm^{-1}
T = 293 K
0.54 × 0.46 × 0.22 mm

Data collection

Bruker APEXII CCD area detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.819, T_{max} = 0.920
8793 measured reflections
1769 independent reflections
1720 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.101
S = 1.20
1769 reflections
119 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6A···O1^{i}	0.93	2.37	3.282 (3)	165
C7—H7A···O4^{ii}	0.96	2.56	3.407 (4)	148

Symmetry codes: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, z$; (ii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL*, *PLATON* (Spek, 2009), *Mercury* and *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5648).

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supplementary materials

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Poly[μ_5-(4-methoxybenzenesulfonato)-sodium]

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1. Comment

Aromatic sulfonic acids are one of several useful sulfonic acids which are frequently used as chemical reagents (King, 1991) such as reagents for phenol preparation. They are also widely used as acid catalysts in organic reactions (Siril *et al.*, 2007) such as for the deprotection of *O*-allylphenols (Babu *et al.*, 2003). Salts of benzenesulfonic acid exhibit pharmaceutical and biological activities (Chanawanno *et al.*, 2010; Taylor *et al.*, 2006), and are also used for nonlinear optical material preparations (Ruanwas *et al.*, 2010) and as raw materials in detergent manufacture (Schöngut *et al.*, 2011). Based on these significant roles played by aromatic sulfonic acids, we have synthesized the sodium salt of 4-methoxybenzenesulfonate and herein we report the crystal structure of the title compound (I).

Within the title coordination polymer there are tetranuclear clusters containing four Na^I ions and four 4-methoxybenzenesulfonate ligands (Fig. 1). All three O atoms of the 4-methoxybenzenesulfonate ligands are involved in coordination to the Na^I ion. The coordination modes of the sulfonate unit are chelating bidentate and bridging monodentate linking two Na^I ions. Each Na^I is in a distorted pentagonal-bipyramidal geometry (Fig. 2) with three pairs of chelating O atoms from the three bidentate sulfonate groups and one bridging O atom from another monodentate sulfonate group which is also coordinated to a symmetry related Na^I ion. The distance of the Na^I ion from the mean plane of the O_5 equatorial atoms is 0.127 Å. Bond lengths (Allen *et al.*, 1987) and angles in the ligand are in normal ranges. The Na—O bond distances in the equatorial plane range from 2.3198 (16) - 2.5585 (17) Å, and the two axial Na—O bond distances are 2.3734 (17) and 2.4637 (16) Å. The O—Na—O bond angles in the equatorial plane are in the range 56.76 (5)–85.88 (6) ° and the axial angle is 158.12 (7)°. These values are comparable to those reported for another Na—O donor complex (Smith *et al.*, 2004). The overall structure is a two-dimensional polymer parallel to (001) (Fig. 3). In addition, weak C—H···O hydrogen bonds (Table 1) link the polymer into a three-dimensional network (Fig. 4).

2. Experimental

To a solution of 4-methoxybenzenesulfonyl chloride (3.00 g, 14.50 mmol) in hot methanol, sodium hydroxide (0.58 g, 14.50 mmol) was added. The suspension was stirred for 1 h. The reaction mixture was then cooled to the room temperature and the resulting white solid formed was filtered off and washed with CH_3OH. Colorless needle-shaped single crystals suitable for X-ray structure determination were recrystallized from a solution of (I) in CH_3OH by slow evaporation at room temperature over a few days.

3. Refinement

All H atoms were fixed geometrically and allowed to ride on their parent atoms, with d(C—H) = 0.93 Å for aromatic and 0.96 for CH_3. The U_{iso} values were constrained to be $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H atoms. A rotating group model was used for the methyl groups.

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008), *PLATON* (Spek, 2009), *Mercury* (Macrae *et al.*, 2006) and *publCIF* (Westrip, 2010).

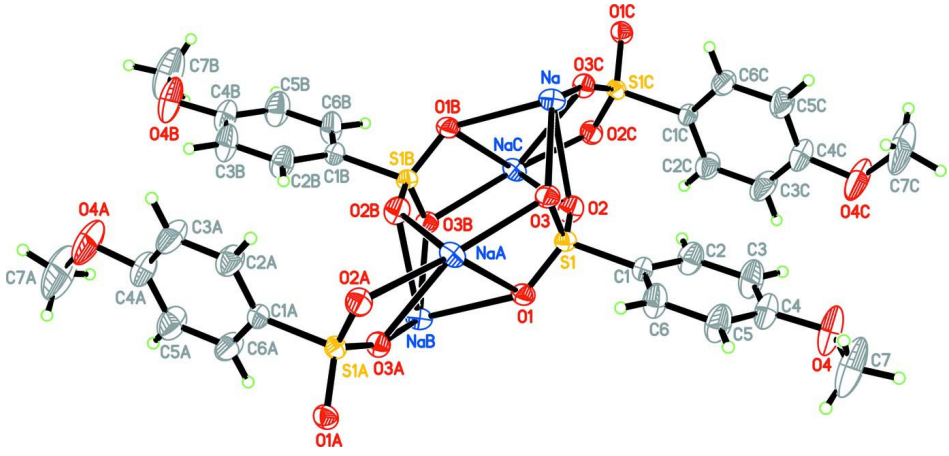

Figure 1

Part of the polymeric structure of (I) showing a tetranuclear cluster with 50% probability displacement ellipsoids. Atoms labelled with the suffix A, B, and C are generated by the symmetry operations (x + 1/2, -y + 1/2, -z + 2), (-x + 1, -y, -z + 2) and (-x + 1/2, y + 1/2, z), respectively.

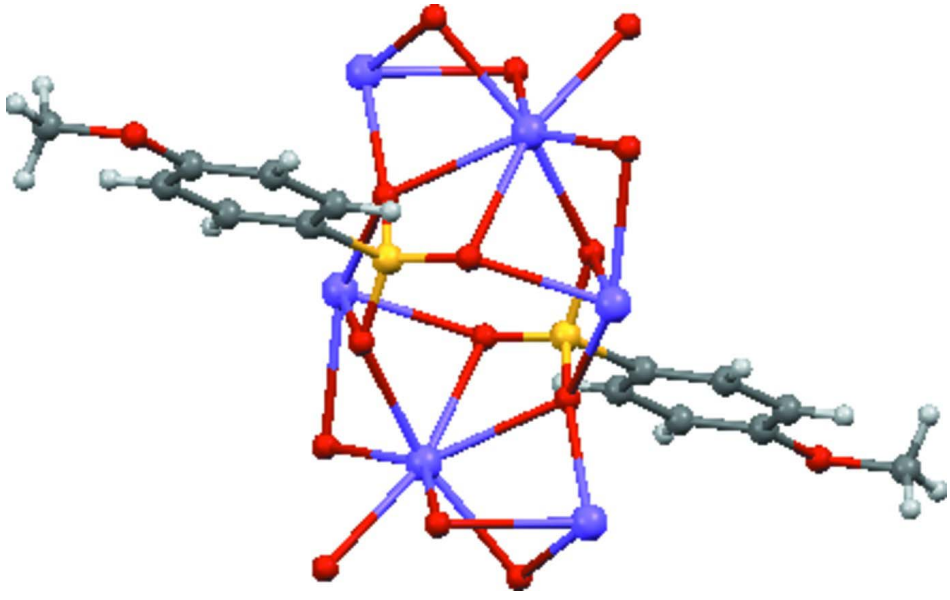

Figure 2

Part of the polymeric structure of (I) showing the coordination environment of Na^{I} ions in (I).

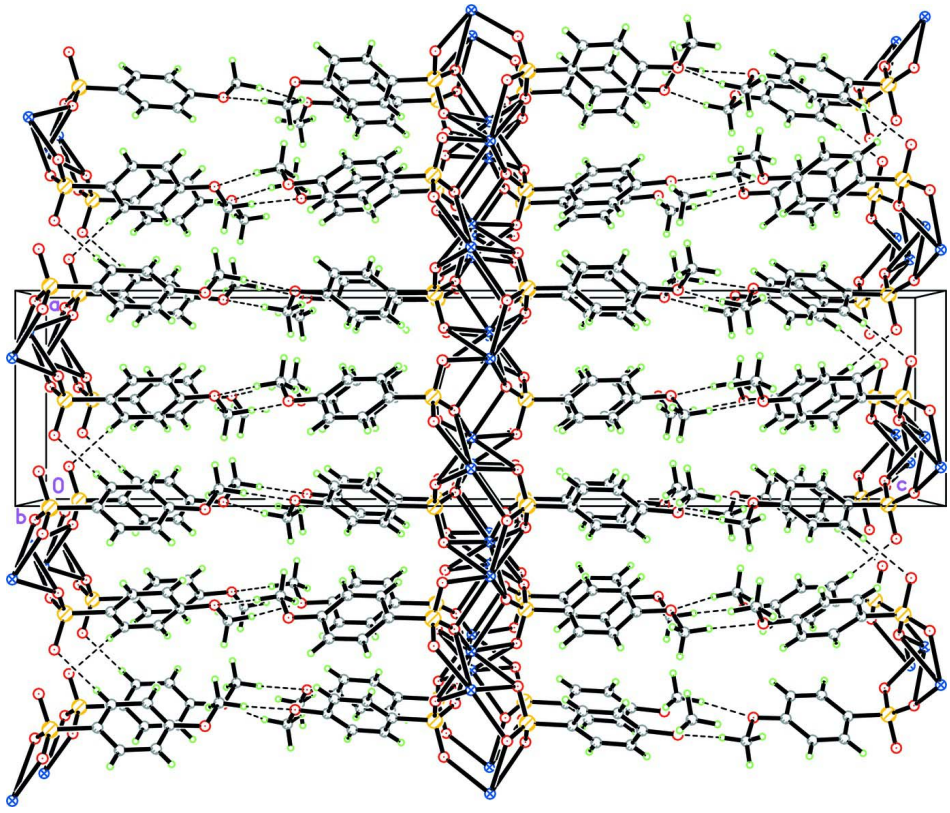

Figure 3

The two-dimensional polymer of (I) viewed along the *b* axis. Hydrogen bonds are drawn as dashed lines.

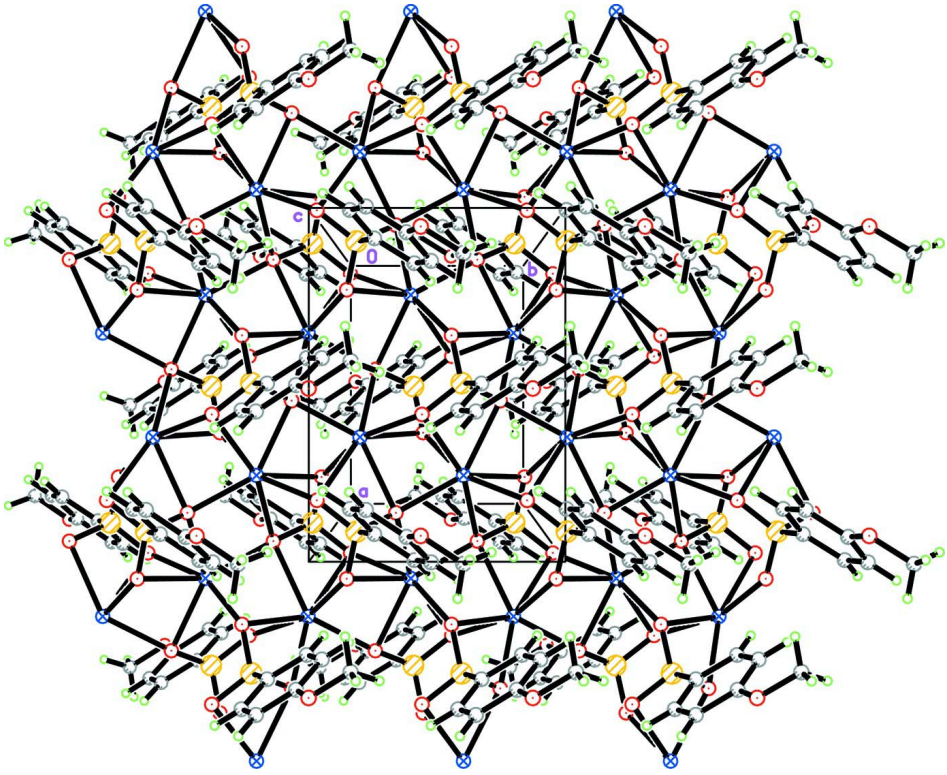

Figure 4

The crystal packing of (I), viewed along the *c* axis.

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Crystal data

[Na($C_7H_7O_4S$)]
M_r = 210.19
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
a = 8.3121 (8) Å
b = 6.0287 (6) Å
c = 35.930 (3) Å
V = 1800.5 (3) Å^3
Z = 8

F(000) = 864
D_x = 1.551 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 1769 reflections
θ = 2.3–26.0°
μ = 0.38 mm^{-1}
T = 293 K
Needle, colorless
0.54 × 0.46 × 0.22 mm

Data collection

Bruker APEXII CCD area detector diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.819, T_{max} = 0.920

8793 measured reflections
1769 independent reflections
1720 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 26.0°, θ_{min} = 2.3°
h = −8→10
k = −7→7
l = −37→44

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.101$
$S = 1.20$
1769 reflections
119 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0372P)^2 + 1.6253P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}
Extinction correction: *SHELXL*, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.042 (3)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.50598 (6)	0.11687 (8)	0.950009 (13)	0.0257 (2)
O1	0.67113 (17)	0.0690 (2)	0.96029 (4)	0.0328 (4)
O2	0.39805 (19)	−0.0717 (3)	0.95165 (4)	0.0386 (4)
O3	0.44483 (18)	0.3026 (2)	0.97215 (4)	0.0324 (4)
O4	0.4881 (4)	0.4270 (4)	0.79459 (6)	0.0843 (8)
C1	0.5047 (2)	0.2071 (4)	0.90315 (6)	0.0300 (5)
C2	0.4151 (4)	0.0971 (4)	0.87675 (7)	0.0483 (6)
H2A	0.3570	−0.0291	0.8831	0.058*
C3	0.4122 (4)	0.1762 (5)	0.84065 (7)	0.0603 (8)
H3A	0.3511	0.1036	0.8227	0.072*
C4	0.4991 (4)	0.3615 (5)	0.83113 (7)	0.0526 (7)
C5	0.5888 (4)	0.4721 (5)	0.85733 (7)	0.0573 (8)
H5A	0.6477	0.5974	0.8508	0.069*
C6	0.5902 (3)	0.3942 (4)	0.89371 (7)	0.0482 (7)
H6A	0.6493	0.4688	0.9118	0.058*
C7	0.5762 (7)	0.6163 (7)	0.78319 (10)	0.1151 (19)
H7A	0.5575	0.6431	0.7572	0.173*
H7B	0.6888	0.5913	0.7873	0.173*
H7C	0.5418	0.7428	0.7973	0.173*
Na	0.18295 (10)	0.12772 (12)	0.98998 (2)	0.0314 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0260 (3)	0.0239 (3)	0.0273 (3)	−0.00035 (18)	0.00168 (17)	0.00130 (18)

O1	0.0280 (7)	0.0355 (8)	0.0349 (8)	0.0061 (6)	0.0021 (6)	0.0032 (6)
O2	0.0435 (9)	0.0347 (8)	0.0376 (8)	−0.0131 (7)	0.0013 (7)	0.0018 (6)
O3	0.0333 (8)	0.0311 (8)	0.0330 (8)	0.0078 (6)	0.0023 (6)	−0.0011 (6)
O4	0.143 (2)	0.0803 (16)	0.0299 (10)	−0.0139 (15)	−0.0124 (11)	0.0134 (10)
C1	0.0332 (11)	0.0318 (11)	0.0250 (10)	−0.0001 (8)	−0.0003 (8)	0.0022 (8)
C2	0.0630 (17)	0.0453 (13)	0.0367 (12)	−0.0158 (12)	−0.0037 (11)	−0.0029 (10)
C3	0.086 (2)	0.0616 (17)	0.0337 (13)	−0.0154 (16)	−0.0139 (13)	−0.0076 (12)
C4	0.077 (2)	0.0512 (16)	0.0294 (13)	0.0020 (14)	−0.0036 (11)	0.0044 (11)
C5	0.078 (2)	0.0531 (15)	0.0404 (13)	−0.0231 (15)	−0.0043 (13)	0.0139 (12)
C6	0.0598 (16)	0.0497 (14)	0.0351 (12)	−0.0218 (12)	−0.0102 (11)	0.0076 (10)
C7	0.210 (6)	0.091 (3)	0.0443 (19)	−0.023 (3)	−0.002 (3)	0.0328 (19)
Na	0.0295 (4)	0.0227 (4)	0.0420 (5)	−0.0004 (3)	0.0039 (3)	0.0000 (3)

Geometric parameters (Å, º)

S1—O2	1.4495 (16)	C3—C4	1.374 (4)
S1—O1	1.4506 (15)	C3—H3A	0.9300
S1—O3	1.4644 (15)	C4—C5	1.374 (4)
S1—C1	1.769 (2)	C5—C6	1.389 (3)
S1—Na^{i}	3.0304 (10)	C5—H5A	0.9300
S1—Na	3.0457 (10)	C6—H6A	0.9300
O1—Na^{ii}	2.4637 (16)	C7—H7A	0.9600
O1—Na^{i}	2.5585 (17)	C7—H7B	0.9600
O2—Na^{iii}	2.3734 (17)	C7—H7C	0.9600
O2—Na	2.5572 (18)	Na—O3^{iii}	2.3198 (16)
O3—Na^{iv}	2.3198 (16)	Na—O2^{iv}	2.3734 (17)
O3—Na^{i}	2.4384 (17)	Na—O3^{v}	2.4384 (17)
O3—Na	2.5021 (17)	Na—O1^{ii}	2.4637 (16)
O4—C4	1.374 (3)	Na—O1^{v}	2.5585 (17)
O4—C7	1.416 (5)	Na—S1^{v}	3.0304 (9)
C1—C6	1.376 (3)	Na—Na^{iv}	3.2138 (6)
C1—C2	1.377 (3)	Na—Na^{iii}	3.2138 (6)
C2—C3	1.382 (4)	Na—Na^{vi}	3.4843 (16)
C2—H2A	0.9300		

O2—S1—O1	114.78 (10)	O2^{iv}—Na—O3	77.09 (6)
O2—S1—O3	111.27 (9)	O3^{v}—Na—O3	140.94 (4)
O1—S1—O3	110.02 (9)	O1^{ii}—Na—O3	87.72 (6)
O2—S1—C1	106.03 (10)	O3^{iii}—Na—O2	76.94 (6)
O1—S1—C1	108.00 (9)	O2^{iv}—Na—O2	104.17 (7)
O3—S1—C1	106.25 (9)	O3^{v}—Na—O2	161.64 (6)
O2—S1—Na^{i}	132.07 (7)	O1^{ii}—Na—O2	79.63 (5)
O1—S1—Na^{i}	57.36 (6)	O3—Na—O2	56.76 (5)
O3—S1—Na^{i}	52.67 (6)	O3^{iii}—Na—O1^{v}	141.19 (6)
C1—S1—Na^{i}	121.58 (8)	O2^{iv}—Na—O1^{v}	81.30 (6)
O2—S1—Na	56.77 (7)	O3^{v}—Na—O1^{v}	57.04 (5)
O1—S1—Na	135.93 (6)	O1^{ii}—Na—O1^{v}	81.74 (5)
O3—S1—Na	54.65 (6)	O3—Na—O1^{v}	84.91 (5)
C1—S1—Na	115.90 (7)	O2—Na—O1^{v}	137.65 (6)
Na^{i}—S1—Na	94.675 (17)	O3^{iii}—Na—S1^{v}	113.81 (5)

S1—O1—Na^{ii}	138.27 (9)	O2^{iv}—Na—S1^{v}	83.53 (4)
S1—O1—Na^{i}	94.12 (7)	O3^{v}—Na—S1^{v}	28.52 (4)
Na^{ii}—O1—Na^{i}	79.55 (5)	O1^{ii}—Na—S1^{v}	88.14 (4)
S1—O2—Na^{iii}	142.94 (10)	O3—Na—S1^{v}	112.98 (4)
S1—O2—Na	94.92 (8)	O2—Na—S1^{v}	164.05 (5)
Na^{iii}—O2—Na	81.26 (5)	O1^{v}—Na—S1^{v}	28.52 (3)
S1—O3—Na^{iv}	162.75 (9)	O3^{iii}—Na—S1	104.79 (5)
S1—O3—Na^{i}	98.81 (8)	O2^{iv}—Na—S1	89.59 (5)
Na^{iv}—O3—Na^{i}	94.12 (6)	O3^{v}—Na—S1	169.25 (5)
S1—O3—Na	96.83 (8)	O1^{ii}—Na—S1	84.13 (4)
Na^{iv}—O3—Na	83.51 (5)	O3—Na—S1	28.52 (3)
Na^{i}—O3—Na	129.48 (6)	O2—Na—S1	28.31 (4)
C4—O4—C7	118.3 (3)	O1^{v}—Na—S1	112.25 (4)
C6—C1—C2	120.3 (2)	S1^{v}—Na—S1	140.75 (3)
C6—C1—S1	118.91 (17)	O3^{iii}—Na—Na^{iv}	162.05 (5)
C2—C1—S1	120.73 (18)	O2^{iv}—Na—Na^{iv}	51.86 (4)
C1—C2—C3	119.3 (2)	O3^{v}—Na—Na^{iv}	96.89 (4)
C1—C2—H2A	120.3	O1^{ii}—Na—Na^{iv}	106.30 (5)
C3—C2—H2A	120.3	O3—Na—Na^{iv}	45.82 (4)
C4—C3—C2	120.3 (2)	O2—Na—Na^{iv}	101.45 (5)
C4—C3—H3A	119.8	O1^{v}—Na—Na^{iv}	48.93 (4)
C2—C3—H3A	119.8	S1^{v}—Na—Na^{iv}	72.048 (19)
C3—C4—C5	120.6 (2)	S1—Na—Na^{iv}	73.41 (3)
C3—C4—O4	115.9 (3)	O3^{iii}—Na—Na^{iii}	50.67 (4)
C5—C4—O4	123.4 (3)	O2^{iv}—Na—Na^{iii}	144.53 (4)
C4—C5—C6	119.0 (2)	O3^{v}—Na—Na^{iii}	116.30 (4)
C4—C5—H5A	120.5	O1^{ii}—Na—Na^{iii}	51.52 (4)
C6—C5—H5A	120.5	O3—Na—Na^{iii}	95.36 (5)
C1—C6—C5	120.3 (2)	O2—Na—Na^{iii}	46.88 (4)
C1—C6—H6A	119.8	O1^{v}—Na—Na^{iii}	133.13 (4)
C5—C6—H6A	119.8	S1^{v}—Na—Na^{iii}	130.16 (2)
O4—C7—H7A	109.5	S1—Na—Na^{iii}	70.98 (3)
O4—C7—H7B	109.5	Na^{iv}—Na—Na^{iii}	139.42 (5)
H7A—C7—H7B	109.5	O3^{iii}—Na—Na^{vi}	44.27 (4)
O4—C7—H7C	109.5	O2^{iv}—Na—Na^{vi}	102.10 (6)
H7A—C7—H7C	109.5	O3^{v}—Na—Na^{vi}	41.61 (4)
H7B—C7—H7C	109.5	O1^{ii}—Na—Na^{vi}	93.85 (5)
O3^{iii}—Na—O2^{iv}	110.78 (7)	O3—Na—Na^{vi}	176.92 (6)
O3^{iii}—Na—O3^{v}	85.88 (6)	O2—Na—Na^{vi}	120.91 (5)
O2^{iv}—Na—O3^{v}	87.82 (6)	O1^{v}—Na—Na^{vi}	97.94 (5)
O3^{iii}—Na—O1^{ii}	91.09 (6)	S1^{v}—Na—Na^{vi}	69.75 (3)
O2^{iv}—Na—O1^{ii}	158.12 (7)	S1—Na—Na^{vi}	149.03 (4)
O3^{v}—Na—O1^{ii}	94.46 (6)	Na^{iv}—Na—Na^{vi}	135.83 (4)
O3^{iii}—Na—O3	133.13 (7)	Na^{iii}—Na—Na^{vi}	83.58 (3)
O2—S1—O1—Na^{ii}	−46.59 (17)	Na^{i}—O3—Na—Na^{iv}	90.00 (8)
O3—S1—O1—Na^{ii}	79.82 (15)	S1—O3—Na—Na^{iii}	30.86 (7)
C1—S1—O1—Na^{ii}	−164.62 (13)	Na^{iv}—O3—Na—Na^{iii}	−166.50 (4)
Na^{i}—S1—O1—Na^{ii}	78.90 (12)	Na^{i}—O3—Na—Na^{iii}	−76.51 (7)

Na—S1—O1—Na^{ii}	20.4 (2)	S1—O2—Na—O3^{iii}	169.52 (8)
O2—S1—O1—Na^{i}	−125.50 (8)	Na^{iii}—O2—Na—O3^{iii}	−47.62 (6)
O3—S1—O1—Na^{i}	0.91 (9)	S1—O2—Na—O2^{iv}	61.03 (8)
C1—S1—O1—Na^{i}	116.48 (9)	Na^{iii}—O2—Na—O2^{iv}	−156.11 (6)
Na—S1—O1—Na^{i}	−58.50 (10)	S1—O2—Na—O3^{v}	−169.45 (17)
O1—S1—O2—Na^{iii}	48.05 (19)	Na^{iii}—O2—Na—O3^{v}	−26.6 (2)
O3—S1—O2—Na^{iii}	−77.71 (18)	S1—O2—Na—O1^{ii}	−96.90 (8)
C1—S1—O2—Na^{iii}	167.19 (15)	Na^{iii}—O2—Na—O1^{ii}	45.95 (5)
Na^{i}—S1—O2—Na^{iii}	−19.4 (2)	S1—O2—Na—O3	−2.80 (6)
Na—S1—O2—Na^{iii}	−82.01 (16)	Na^{iii}—O2—Na—O3	140.06 (7)
O1—S1—O2—Na	130.06 (8)	S1—O2—Na—O1^{v}	−31.57 (12)
O3—S1—O2—Na	4.30 (10)	Na^{iii}—O2—Na—O1^{v}	111.29 (8)
C1—S1—O2—Na	−110.81 (8)	S1—O2—Na—S1^{v}	−56.4 (2)
Na^{i}—S1—O2—Na	62.61 (10)	Na^{iii}—O2—Na—S1^{v}	86.49 (17)
O2—S1—O3—Na^{iv}	−94.5 (3)	Na^{iii}—O2—Na—S1	142.86 (10)
O1—S1—O3—Na^{iv}	137.1 (3)	S1—O2—Na—Na^{iv}	7.82 (8)
C1—S1—O3—Na^{iv}	20.5 (4)	Na^{iii}—O2—Na—Na^{iv}	150.67 (4)
Na^{i}—S1—O3—Na^{iv}	138.1 (4)	S1—O2—Na—Na^{iii}	−142.86 (10)
Na—S1—O3—Na^{iv}	−90.1 (3)	S1—O2—Na—Na^{vi}	174.81 (6)
O2—S1—O3—Na^{i}	127.40 (8)	Na^{iii}—O2—Na—Na^{vi}	−42.33 (7)
O1—S1—O3—Na^{i}	−0.97 (10)	O2—S1—Na—O3^{iii}	−10.56 (9)
C1—S1—O3—Na^{i}	−117.63 (8)	O1—S1—Na—O3^{iii}	−103.07 (11)
Na—S1—O3—Na^{i}	131.81 (8)	O3—S1—Na—O3^{iii}	174.35 (10)
O2—S1—O3—Na	−4.41 (10)	C1—S1—Na—O3^{iii}	82.24 (9)
O1—S1—O3—Na	−132.77 (7)	Na^{i}—S1—Na—O3^{iii}	−149.16 (5)
C1—S1—O3—Na	110.56 (8)	O2—S1—Na—O2^{iv}	−121.97 (9)
Na^{i}—S1—O3—Na	−131.81 (8)	O1—S1—Na—O2^{iv}	145.51 (10)
O2—S1—C1—C6	176.20 (19)	O3—S1—Na—O2^{iv}	62.94 (8)
O1—S1—C1—C6	−60.3 (2)	C1—S1—Na—O2^{iv}	−29.17 (9)
O3—S1—C1—C6	57.7 (2)	Na^{i}—S1—Na—O2^{iv}	99.43 (5)
Na^{i}—S1—C1—C6	1.9 (2)	O2—S1—Na—O3^{v}	162.0 (3)
Na—S1—C1—C6	115.82 (19)	O1—S1—Na—O3^{v}	69.5 (3)
O2—S1—C1—C2	−1.4 (2)	O3—S1—Na—O3^{v}	−13.1 (3)
O1—S1—C1—C2	122.1 (2)	C1—S1—Na—O3^{v}	−105.2 (3)
O3—S1—C1—C2	−119.9 (2)	Na^{i}—S1—Na—O3^{v}	23.4 (3)
Na^{i}—S1—C1—C2	−175.71 (18)	O2—S1—Na—O1^{ii}	79.02 (9)
Na—S1—C1—C2	−61.8 (2)	O1—S1—Na—O1^{ii}	−13.49 (13)
C6—C1—C2—C3	0.2 (4)	O3—S1—Na—O1^{ii}	−96.07 (8)
S1—C1—C2—C3	177.8 (2)	C1—S1—Na—O1^{ii}	171.82 (9)
C1—C2—C3—C4	0.6 (5)	Na^{i}—S1—Na—O1^{ii}	−59.58 (4)
C2—C3—C4—C5	−0.6 (5)	O2—S1—Na—O3	175.09 (11)
C2—C3—C4—O4	−179.9 (3)	O1—S1—Na—O3	82.58 (12)
C7—O4—C4—C3	−179.6 (4)	C1—S1—Na—O3	−92.11 (11)
C7—O4—C4—C5	1.2 (5)	Na^{i}—S1—Na—O3	36.49 (7)
C3—C4—C5—C6	−0.1 (5)	O1—S1—Na—O2	−92.51 (12)
O4—C4—C5—C6	179.1 (3)	O3—S1—Na—O2	−175.09 (11)
C2—C1—C6—C5	−0.9 (4)	C1—S1—Na—O2	92.80 (11)
S1—C1—C6—C5	−178.6 (2)	Na^{i}—S1—Na—O2	−138.60 (8)
C4—C5—C6—C1	0.9 (5)	O2—S1—Na—O1^{v}	157.60 (9)

S1—O3—Na—O3^{iii}	−7.49 (14)	O1—S1—Na—O1^{v}	65.09 (12)
Na^{iv}—O3—Na—O3^{iii}	155.15 (6)	O3—S1—Na—O1^{v}	−17.49 (8)
Na^{i}—O3—Na—O3^{iii}	−114.86 (10)	C1—S1—Na—O1^{v}	−109.60 (9)
S1—O3—Na—O2^{iv}	−113.99 (8)	Na^{i}—S1—Na—O1^{v}	19.00 (4)
Na^{iv}—O3—Na—O2^{iv}	48.64 (6)	O2—S1—Na—S1^{v}	158.80 (9)
Na^{i}—O3—Na—O2^{iv}	138.64 (9)	O1—S1—Na—S1^{v}	66.29 (11)
S1—O3—Na—O3^{v}	176.15 (9)	O3—S1—Na—S1^{v}	−16.29 (8)
Na^{iv}—O3—Na—O3^{v}	−21.21 (9)	C1—S1—Na—S1^{v}	−108.40 (9)
Na^{i}—O3—Na—O3^{v}	68.79 (11)	Na^{i}—S1—Na—S1^{v}	20.20 (4)
S1—O3—Na—O1^{ii}	81.88 (7)	O2—S1—Na—Na^{iv}	−172.01 (8)
Na^{iv}—O3—Na—O1^{ii}	−115.49 (5)	O1—S1—Na—Na^{iv}	95.48 (10)
Na^{i}—O3—Na—O1^{ii}	−25.49 (8)	O3—S1—Na—Na^{iv}	12.91 (7)
S1—O3—Na—O2	2.78 (6)	C1—S1—Na—Na^{iv}	−79.21 (8)
Na^{iv}—O3—Na—O2	165.42 (7)	Na^{i}—S1—Na—Na^{iv}	49.40 (2)
Na^{i}—O3—Na—O2	−104.59 (9)	O2—S1—Na—Na^{iii}	27.79 (8)
S1—O3—Na—O1^{v}	163.79 (7)	O1—S1—Na—Na^{iii}	−64.73 (10)
Na^{iv}—O3—Na—O1^{v}	−33.58 (5)	O3—S1—Na—Na^{iii}	−147.30 (7)
Na^{i}—O3—Na—O1^{v}	56.42 (8)	C1—S1—Na—Na^{iii}	120.59 (8)
S1—O3—Na—S1^{v}	168.89 (5)	Na^{i}—S1—Na—Na^{iii}	−110.811 (19)
Na^{iv}—O3—Na—S1^{v}	−28.48 (6)	O2—S1—Na—Na^{vi}	−8.67 (11)
Na^{i}—O3—Na—S1^{v}	61.52 (8)	O1—S1—Na—Na^{vi}	−101.19 (12)
Na^{iv}—O3—Na—S1	162.63 (10)	O3—S1—Na—Na^{vi}	176.24 (12)
Na^{i}—O3—Na—S1	−107.37 (11)	C1—S1—Na—Na^{vi}	84.13 (12)
S1—O3—Na—Na^{iv}	−162.63 (10)	Na^{i}—S1—Na—Na^{vi}	−147.27 (9)

Symmetry codes: (i) *x*+1/2, −*y*+1/2, −*z*+2; (ii) −*x*+1, −*y*, −*z*+2; (iii) −*x*+1/2, *y*−1/2, *z*; (iv) −*x*+1/2, *y*+1/2, *z*; (v) *x*−1/2, −*y*+1/2, −*z*+2; (vi) −*x*, −*y*, −*z*+2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6*A*···O1^{vii}	0.93	2.37	3.282 (3)	165
C7—H7*A*···O4^{viii}	0.96	2.56	3.407 (4)	148

Symmetry codes: (vii) −*x*+3/2, *y*+1/2, *z*; (viii) −*x*+1, *y*+1/2, −*z*+3/2.